

2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.14e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.32e-01

Confidence level: 6.20e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2,4-Trimethyl-1,3-pentanediol</div> <div>Measured: 1.30e-01</div> <div>Predicted: 2.14e-01</div>	<div>Image not found</div> <div>Prenderol</div> <div>Measured: 1.51</div> <div>Predicted: 1.04</div>	<div>Image not found</div> <div>Terpin</div> <div>Measured: 2.06e-02</div> <div>Predicted: 3.89e-02</div>
<div>Image not found</div> <div>Terpin</div> <div>Measured: 2.06e-02</div> <div>Predicted: 3.89e-02</div>	<div>Image not found</div> <div>2-Methyl-2,4-pentanediol</div> <div>Measured: 8.46</div> <div>Predicted: 3.58</div>	